Integrating uncertainty in model parameters, input, and model structure in watershed modeling

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TEXAS A&M AGRILIFE RESEARCH

Background

- **Prevailing modeling practice**

  - rely on a single model

  - consider only parameter uncertainty (parameter calibration)

- **Multiple model structures**

  - tremendous amount of resources invested in developing more models

  - simplified assumptions and mathematical representations

  - no particular model is superior for all type of applications and under all conditions

- **Input error model**

  - account for rainfall uncertainty

Research Goal

- Develop a procedure for integrating model parameter, input, and structural uncertainty for model calibration and uncertainty analysis

- Extend APEX-CUTE's capability by incorporating
  - An input error model
  - Bayesian model averaging (BMA) and
  - Dynamically dimensioned search – approximation of uncertainty (DDS-AU)

APEX: Agricultural Policy Environmental eXtender

Can be configured for:

- Irrigation, furrow diking, buffer strips, terraces, waterways, fertilization, manure management, lagoons, crop rotation and selection, pesticide application, grazing, and tillage
- Routing of water, sediment, nutrient, and pesticide

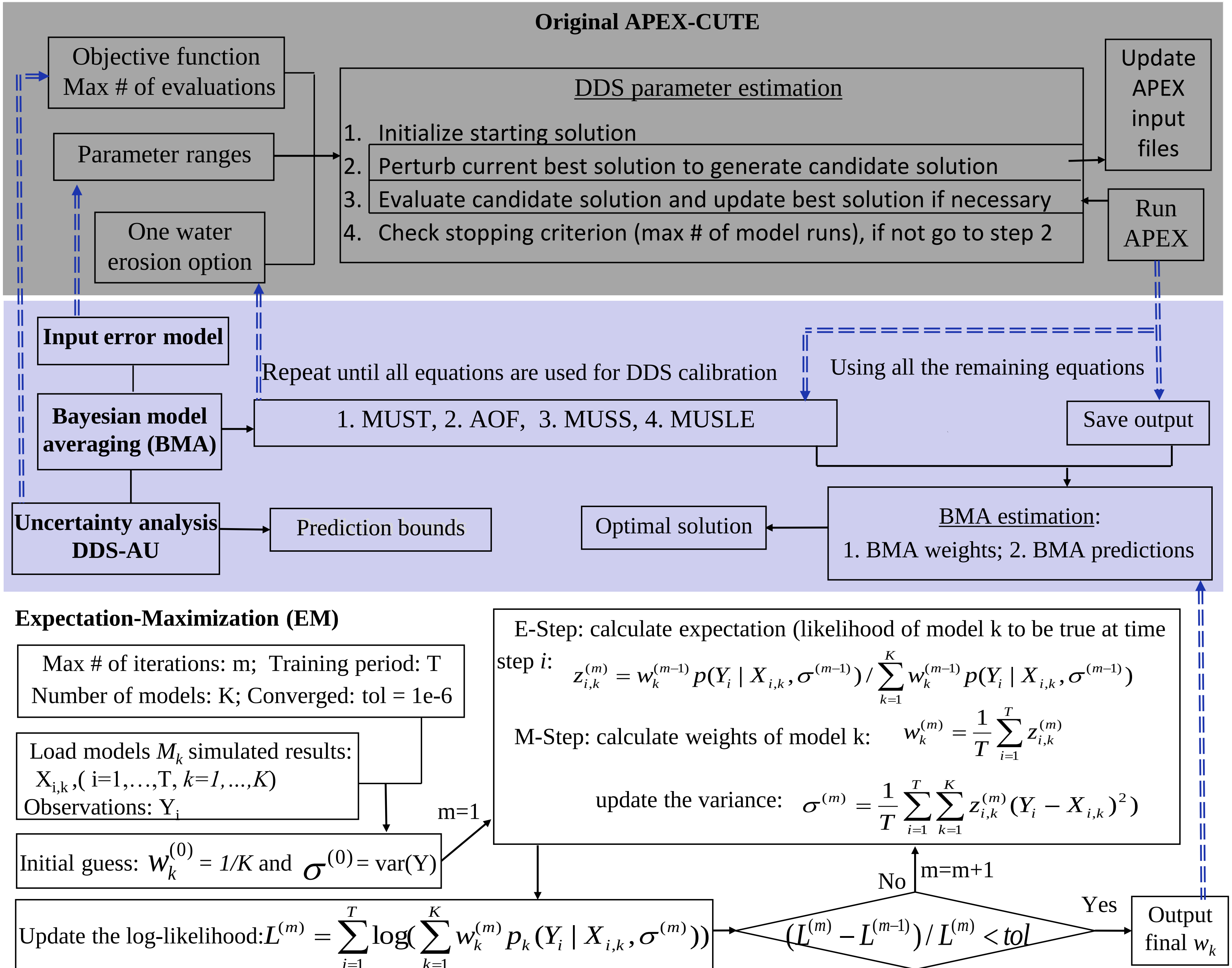
Water Erosion Method	Formula
General formula	$Y = X \times EK \times CVF \times PE \times SL \times ROKF$
(1) Modified USLE (MUSLE)	$X = 1.586(Qq_p)^{0.56} A^{0.12}$
(2) MUSLE variation 1 (MUST)	$X = 2.5(Qq_p)^{0.5}$
(3) MUSLE variation 2 (MUSS)	$X = 0.79(Qq_p)^{0.65} A^{0.009}$
(4) Onstad-Foster modification of USLE (AOF)	$X = 0.646 EI_{30} + 0.45(Qq_p)^{0.33}$

Original **APEX-CUTE** (recently developed): APEX auto-calibration tool (Wang et al., 2014)

- accounted for parameter uncertainty only,
- used the <u>dynamically dimensioned search (DDS)</u> algorithm

Dynamically dimensioned search (DDS) (Tolson and Shoemaker, 2007,WRR)

- fast approximate stochastic global optimization algorithm
- search scaled to pre-specified max # of function evaluations (global search at the beginning and more localized in the end)
- perturbation magnitudes are randomly sampled from a normal distribution with a mean of zero.


Original APEX-CUTE
Objective function
Max # of evaluations
Parameter ranges
One water erosion option
DDS parameter estimation
1. Initialize starting solution
2. Perturb current best solution to generate candidate solution
3. Evaluate candidate solution and update best solution if necessary
4. Check stopping criterion (max # of model runs), if not go to step 2
Update APEX input files
Run APEX
Input error model
Bayesian model averaging (BMA)
Uncertainty analysis DDS-AU
Repeat until all equations are used for DDS calibration
Using all the remaining equations
1. MUST, 2. AOF, 3. MUSS, 4. MUSLE
Save output
Prediction bounds
Optimal solution
BMA estimation:
1. BMA weights; 2. BMA predictions
Expectation-Maximization (EM)
Max # of iterations: m; Training period: T
Number of models: K; Converged: tol = 1e-6
Load models M_k simulated results:
$X_{i,k}$,(i=1,…,T, $k=1,…,K$)
Observations: Y_i
Initial guess: $w_k^{(0)} = 1/K$ and $\sigma^{(0)} = \mathrm{var}(Y)$
m=1
E-Step: calculate expectation (likelihood of model k to be true at time step i:
$z_{i,k}^{(m)} = w_k^{(m-1)} p(Y_i \mid X_{i,k}, \sigma^{(m-1)}) / \sum_{k=1}^{K} w_k^{(m-1)} p(Y_i \mid X_{i,k}, \sigma^{(m-1)})$
M-Step: calculate weights of model k: $w_k^{(m)} = \frac{1}{T} \sum_{i=1}^{T} z_{i,k}^{(m)}$
update the variance: $\sigma^{(m)} = \frac{1}{T} \sum_{i=1}^{T} \sum_{k=1}^{K} z_{i,k}^{(m)} (Y_i - X_{i,k})^2)$
Update the log-likelihood: $L^{(m)} = \sum_{i=1}^{T} \log(\sum_{k=1}^{K} w_k^{(m)} p_k (Y_i \mid X_{i,k}, \sigma^{(m)}))$
$(L^{(m)} - L^{(m-1)}) / L^{(m)} < tol$
No
m=m+1
Yes
Output final w_k

Input error model

The rainfall uncertainty was considered using an input error model which assumes a random Gaussian error as a multiplier for each input rainfall observation as proposed by Ajami et al. (2007) (WRR):

$$\overline{R}_t = \phi_t R_t \,; \qquad \phi \sim N\left(m, \sigma_m^2\right)$$

$\overline{R}_t$: true rainfall depth at time *t*;

R_t : observed rainfall depth at time *t*;

ϕ_t : represents a random multiplier (noise) at time *t* with mean *m*, $m \in [0.9, 1.1]$ and variance σ_m^2, $\sigma_m^2 \in [10^{-5}, 10^{-3}]$

	Influential input or parameter	Description	Range	Default	Chosen in the case study (1: yes; 0: no)*
APEX	CN2 (If Curve Number method used)	Initial condition II curve number (CN2) or landuse number (LUN)	± 5	-	1
	Parm20	Runoff curve number initial abstraction	0.05 – 0.4	0.2	1
	Parm46	RUSLE c factor coefficient in exponential residue function in residue factor	0.5 - 1.5	0.5	1
	…….	…….	…….	…….	…….
Input error model	m	Rainfall depth multiplier normal distribution mean	0.9 – 1.1	0.9	1
	σ_m	Rainfall depth multiplier normal distribution variance (in e-2)	0.001 – 0.1	0.001	1

Bayesian model averaging (BMA)

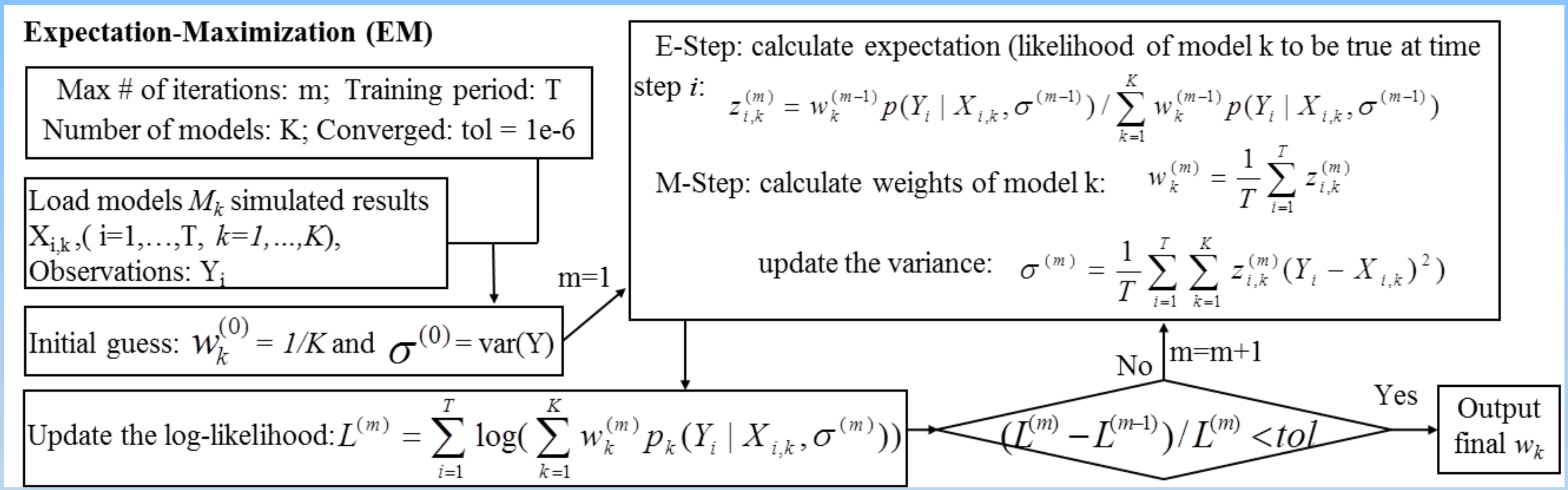
Bayesian theorem is applied over a set of considered models, $M_{k,}$ to calculate a weighted probability distribution $p(y)$ for model output:

$$p(y) = \sum_{k=1}^{m} p\left(M_k \mid Y^T\right) p\left(y_k \mid M_k\right) = \sum_{k=1}^{m} w_k\left(y_k \mid M_k\right)$$

$p(y)$: weighted output distribution based on M_k considered models;

$p(M_k \mid Y^T)$: posterior probability of model M_k being correct model given the training data Y^T, and it reflects how well model M_k fits the observed variable during the training period T, and it is also known as the BMA weight w_k.

$p(y_k \mid M_k)$: forecast pdf of output variable y_k based on model $M_{k.}$



DDS–approximation of uncertainty (DDS-AU)

- Proposed by Tolson & Shoemaker (2008), WRR.
- Relies on DDS optimization where multiple independent optimization trials (each with a relatively small number of model evaluations) are used to independently identify multiple acceptable or behavioral model parameter sets.
- Termed an approximation because it uses a pseudolikelihood function (Nash–Sutcliffe efficiency, root mean square error, or aggregated statistics criterions) rather than a statistically rigorous likelihood function.
- Prediction bounds are constructed as the maximum and minimum values of the output among behavior runs.

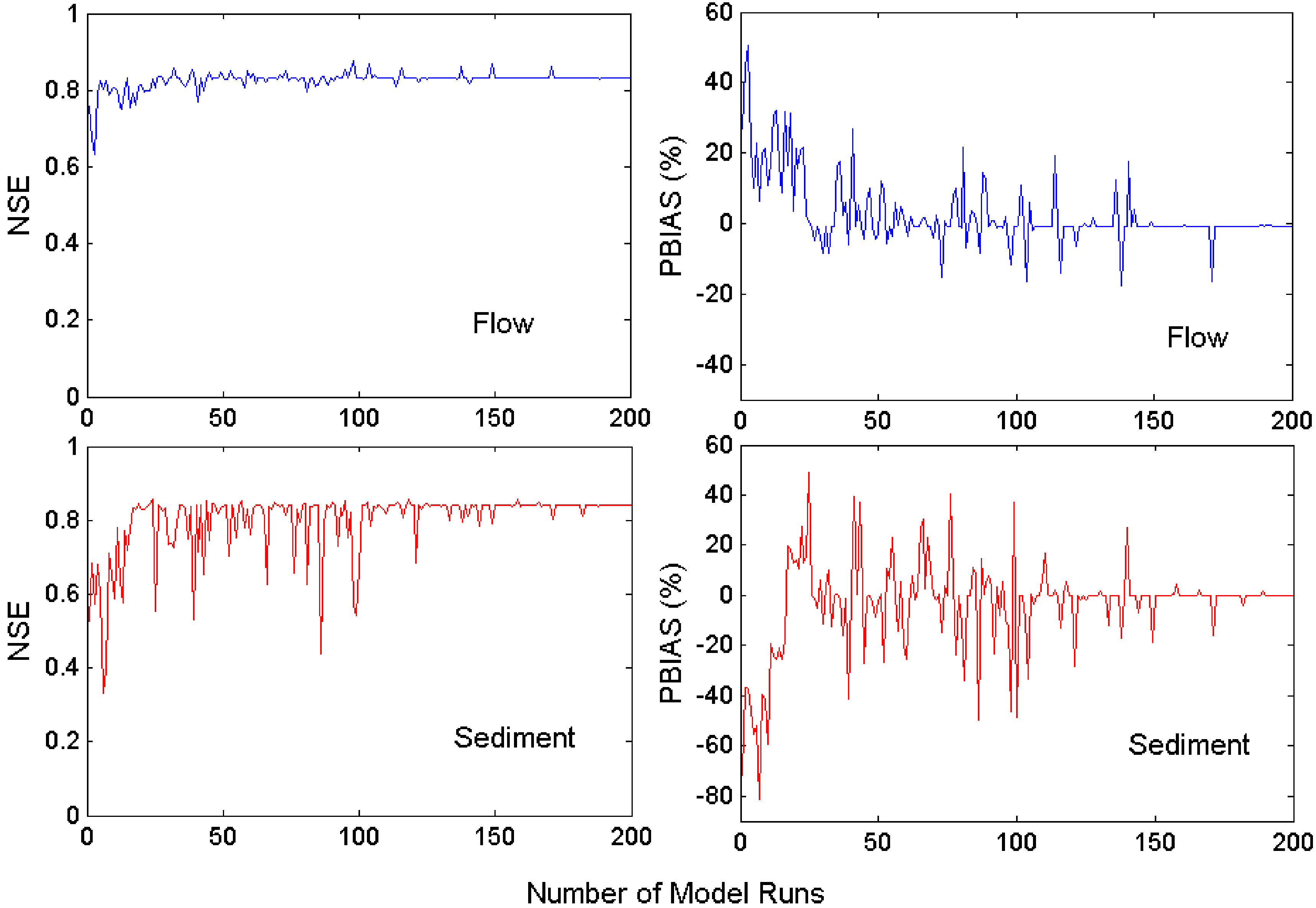
$$F = \sum_{i=1}^{k} w_i \times OF_i$$

$$OF_i = \left((1 - NSE_i)^2 + \left(\left| PBIAS_i \right| + 0.5 \right)^2 \right)^{1/2}$$

where k is total number of interested prediction/output variables for calibration, e.g., if both streamflow and sediment yield are to be calibrated, then k is equal to 2;

w_i is the weight assigned for the portion of the output variable i performance;

OF is designed to maximize *NSE* and reduce |*PBIAS*| values.

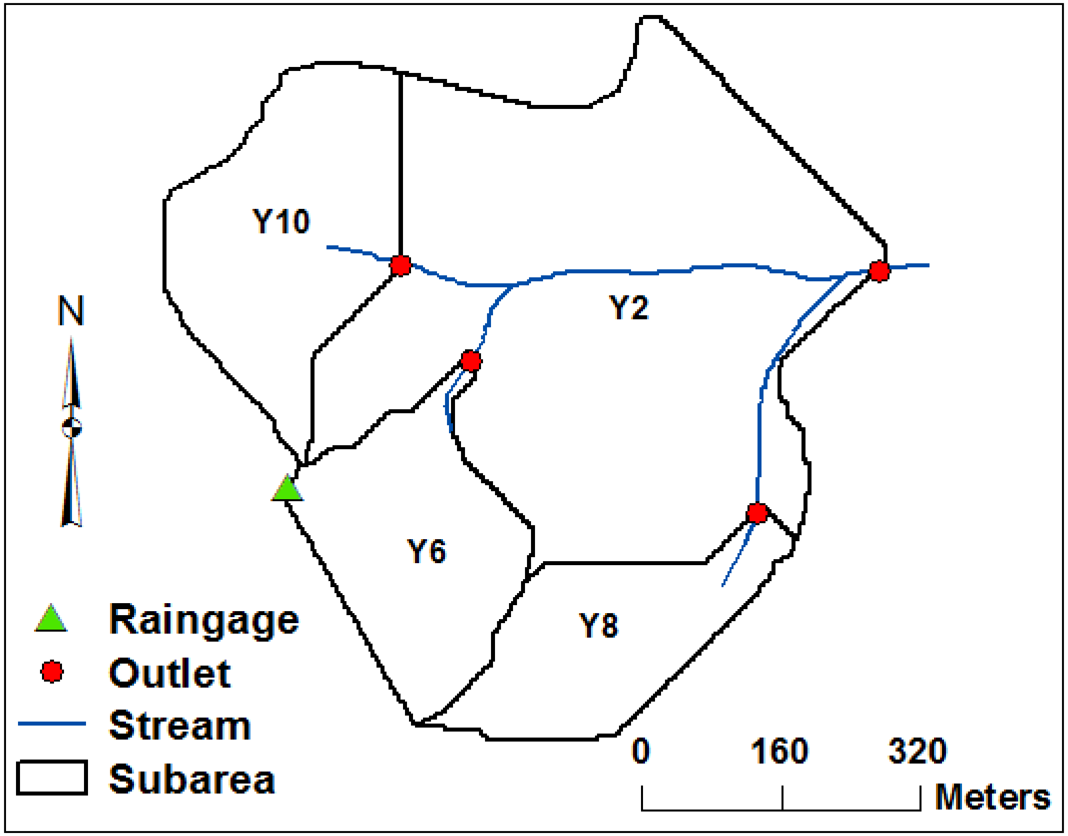


NSE
PBIAS (%)
Flow
Sediment
Number of Model Runs
0
50
100
150
200
0.2
0.4
0.6
0.8
1
60
40
20
-20
-40
-60
-80

Case Study

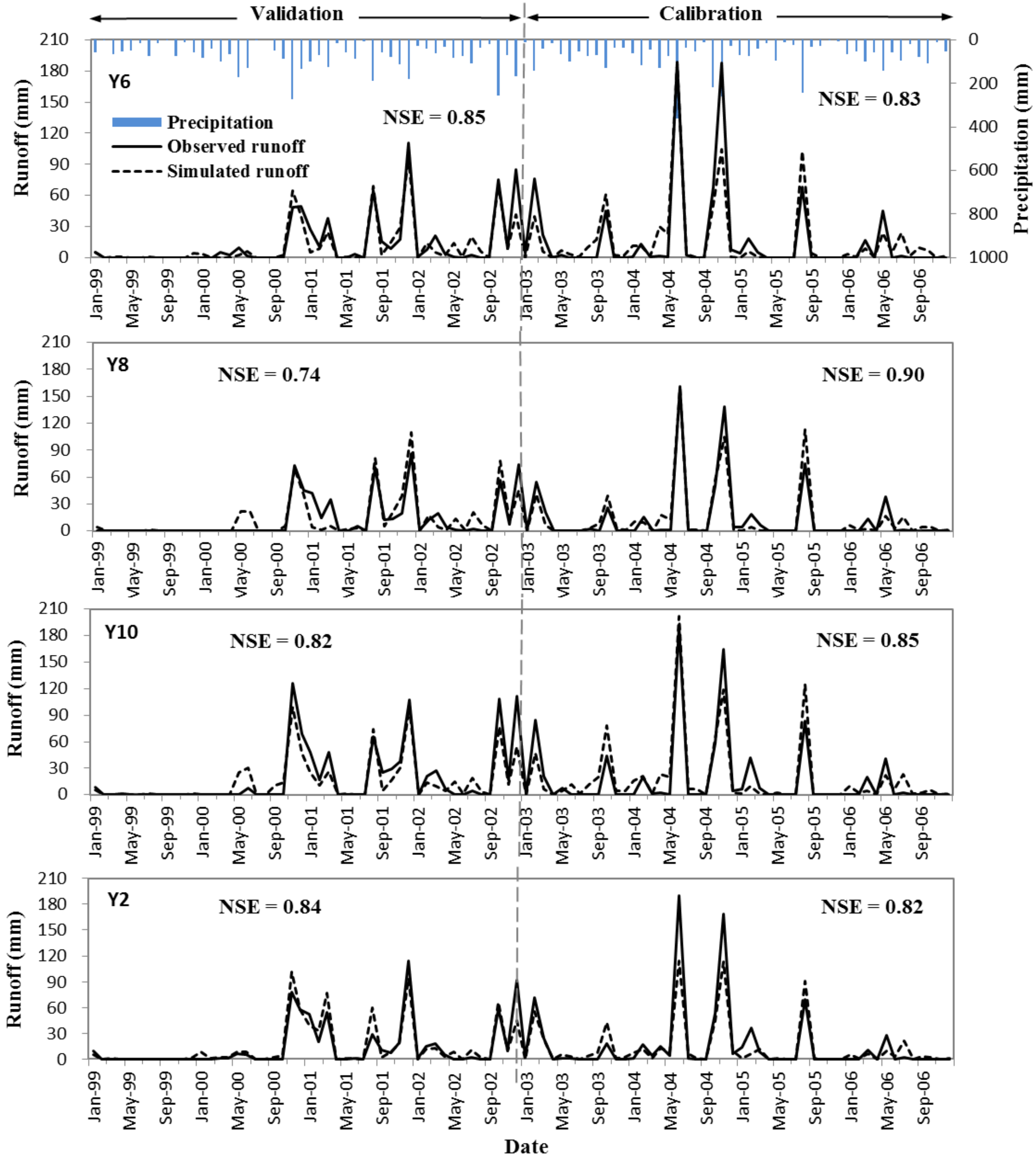
USDA-Agricultural Research Service (ARS) Grassland, Soil and Water Research Laboratory experimental watershed (44 ha) near Riesel, Texas

- Soil: Houston Black clay (fine, smectitic, thermic Udic Haplusterts)
- Y6, Y8, and Y10: arable cultivated fields, terraced and planted on the contour, corn, winter wheat, sorghum, and oats rotation
- Y2: rangeland
- Annual precipitation ranged from 470~1400 mm during study period (1999-2006).



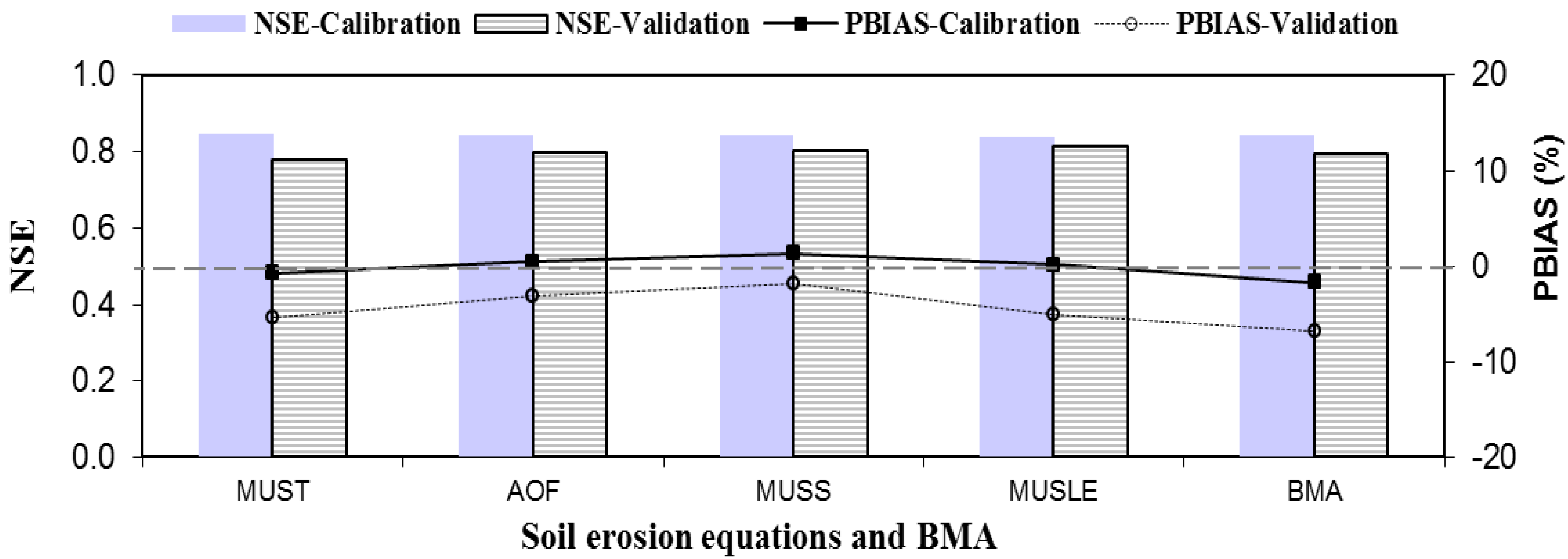
Results
- Flow

Monthly observed & simulated flow based on calibration of the MUST erosion method



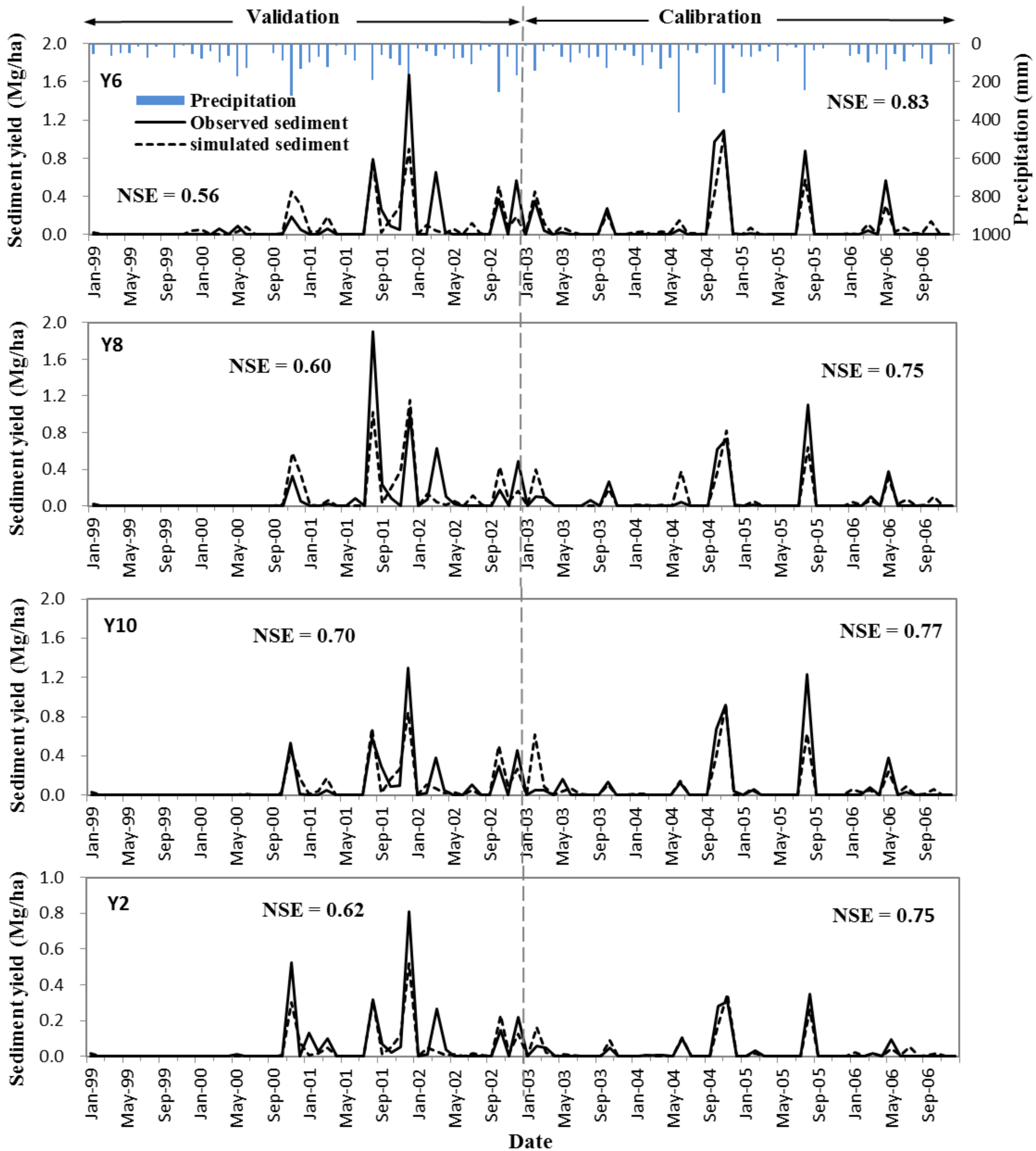
Results
- Flow

Nash-Sutcliffe efficiency (NSE) and average percent error (PBIAS) of flow at the Y2 watershed outlet based on individual erosion method calibration and BMA prediction

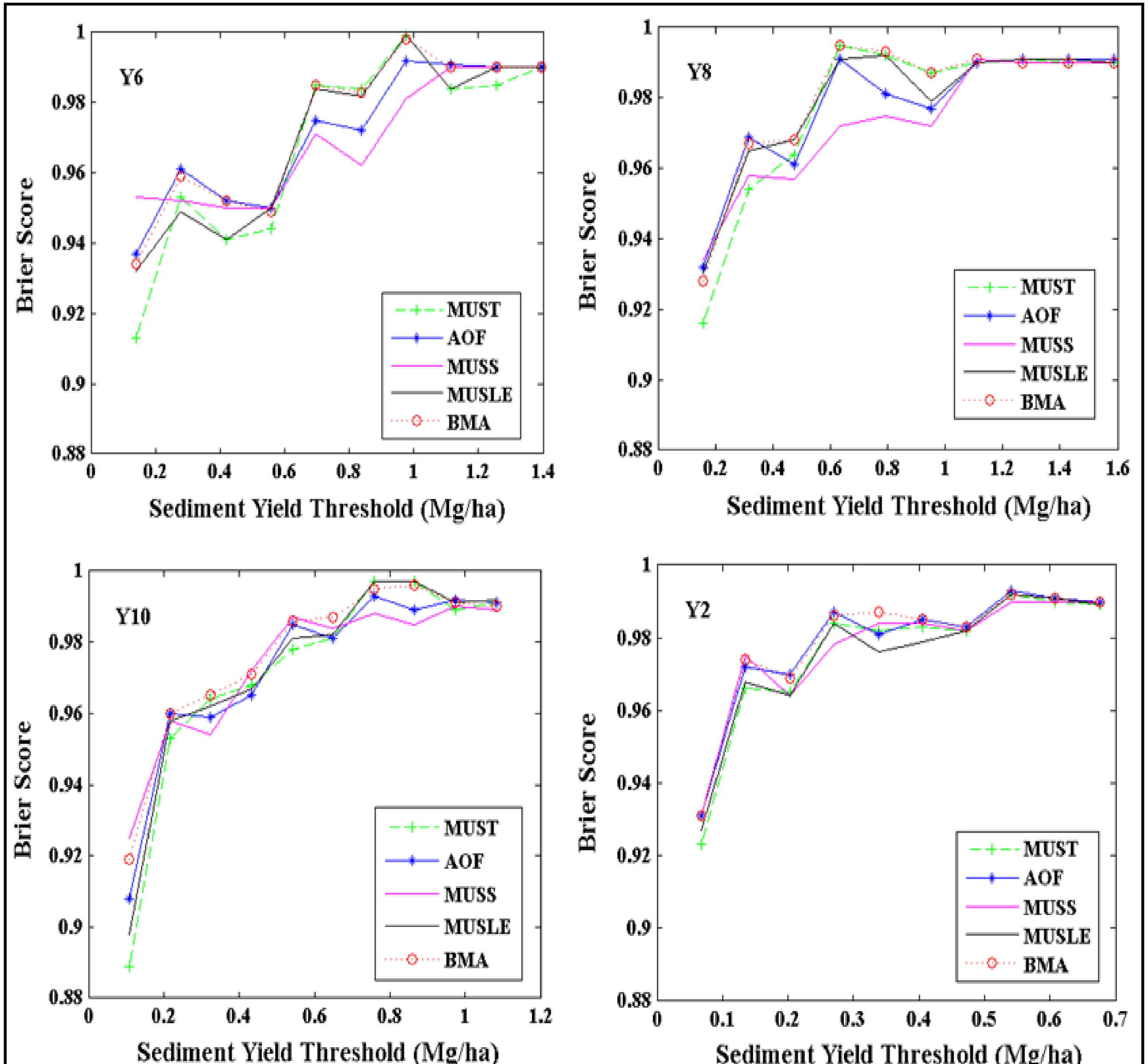


- Sediment

Monthly observed and BMA predictions of sediment for calibration and validation periods.

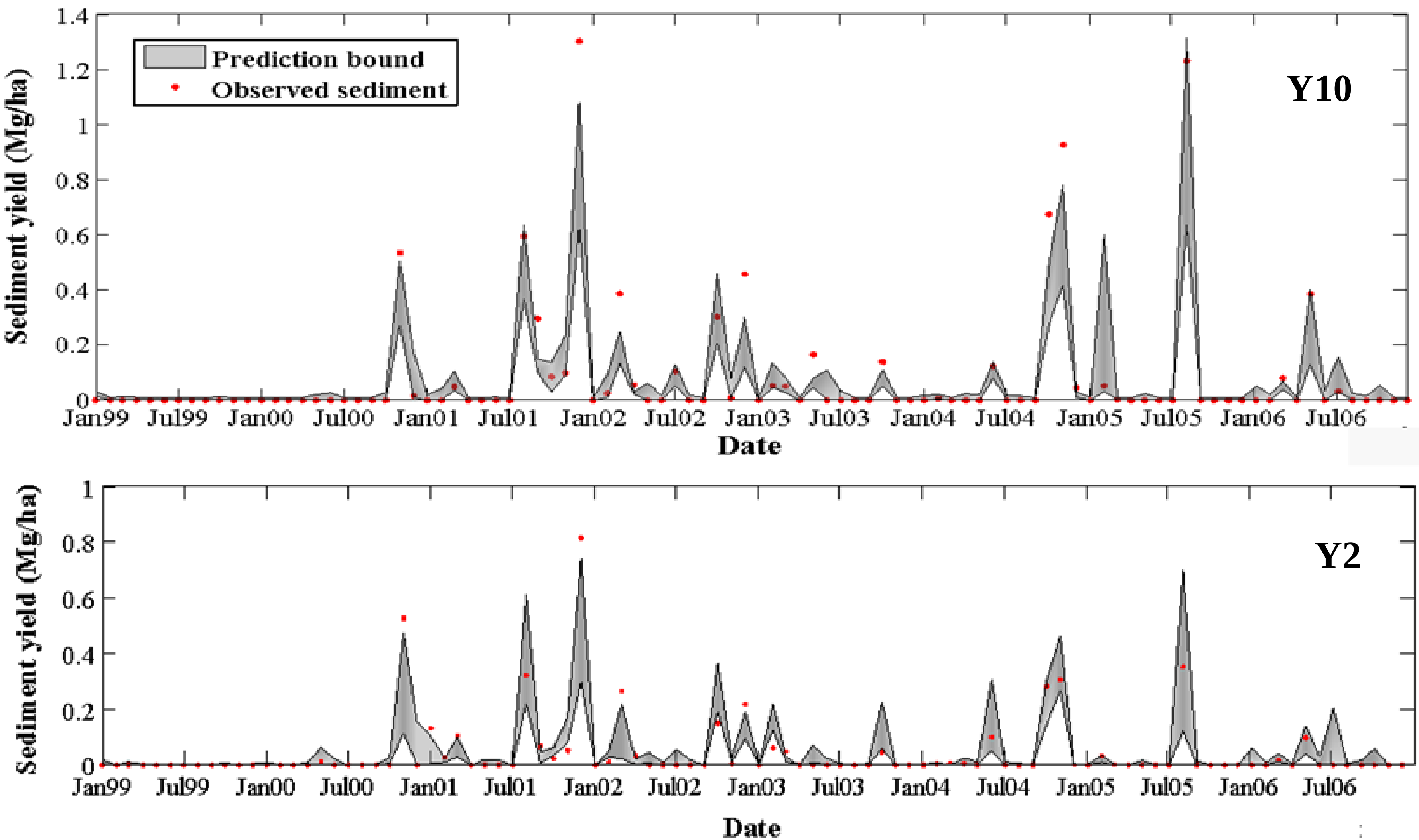


Brier score to compare simulation skill of each erosion method and BMA technique



The higher score indicates the frequency of simulated target event is closer to the corresponding observed frequency, therefore higher BS values represents better simulation skill.

Monthly sediment prediction bound based on BMA predictions



Conclusions

- The extended APEX-CUTE is a computationally efficient and flexible tool.
- Monthly flow and sediment yields resulted in satisfactory model performance.
- BMA predictions have relatively higher Brier scores in most of the sediment yield regimes (10 intervals) than individual methods, and also resulted in narrower prediction bounds.
- The results were limited in one watershed based on four erosion methods within APEX, yet the approach provides opportunity to better account modeling uncertainty where multi-models are available.

Thank You!

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